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16 **Keywords**

17 Stylolite, Permeability, Compaction, Classification, Zechstein, Reservoir
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20 **Abstract**

21 We modeled the geometrical roughening of bedding-parallel, mainly layer-
22 dominated stylolites in order to understand their structural evolution, to present
23 an advanced classification of stylolite shapes and to relate this classification to
24 chemical compaction and permeability variations at stylolites. Stylolites are
25 rough dissolution seams that develop in sedimentary basins during chemical
26 compaction. In the Zechstein 2 carbonate units, an important lean gas reservoir
27 in the southern Permian Zechstein basin in Germany, stylolites influence local
28 fluid flow, mineral replacement reactions and hence the permeability of the
29 reservoir. Our simulations demonstrate that layer-dominated stylolites can
30 grow in three distinct stages: an initial slow nucleation phase, a fast layer-
31 pinning phase and a final freezing phase if the layer is completely dissolved
32 during growth. Dissolution of the pinning layer and thus destruction of the
33 stylolite's compaction tracking capabilities is a function of the background noise
34 in the rock and the dissolution rate of the layer itself. Low background noise
35 needs a slower dissolving layer for pinning to be successful but produces flatter
36 teeth than higher background noise. We present an advanced classification based
37 on our simulations and separate stylolites into four classes: (1) rectangular layer
38 type, (2) seismogram pinning type, (3) suture/sharp peak type and (4) simple
39 wave-like type. Rectangular layer type stylolites are the most appropriate for
40 chemical compaction estimates because they grow linearly and record most of
41 the actual compaction (up to 40mm in the Zechstein example). Seismogram
42 pinning type stylolites also provide good tracking capabilities, with the largest
43 teeth tracking most of the compaction. Suture/sharp peak type stylolites grow in
44 a non-linear fashion and thus do not record most of the actual compaction.
45 However, when a non-linear growth law is used, the compaction estimates are
46 similar to those making use of the rectangular layer type stylolites. Simple wave-
47 like stylolites are not useful for compaction estimates, since their growth is
48 highly non-linear with a very low growth exponent. Stylolites can produce seals
49 if they are collecting sealing material or they can intensify sealing capabilities of

pinning layers. However, the development of teeth and spikes offsets and thus destroys continuous stylolite layers so that the permeability across the stylolite becomes very heterogeneous and they are not sealing. Rectangular layer and seismogram pinning type stylolites intensify local seals at teeth tips but destroy sealing capabilities of layers by offsetting them, so that fluid fluxes across these structures will be very heterogeneous. Suture/sharp peak stylolites can create seals if they collect enough sealing material, however, if the collecting material does not seal or if spikes offset the sealing material the stylolite leaks. We propose that our classification can be used to realistically estimate chemical compaction in reservoirs and gives an indication on how heterogeneous fluids will travel across stylolites.

1 Introduction

Stylolites are rough or wavy dissolution seams (Fig. 1) that develop during localized intergranular pressure solution (Stockdale, 1922; Dunnington, 1954; Park and Schot, 1968; Merino, 1992; Railsback, 1993; Gratier et al., 2005). They are visible in rocks because the stylolite collects material that dissolves slower than the host rock, and this material often has a dark color (because it typically contains clay, mica, oxides). Stylolites are very common in rocks that have undergone diagenesis (sedimentary stylolites parallel to bedding) or tectonic strain (tectonic stylolites that are usually at an angle to bedding). Limestones are very prone to be strongly affected by stylolites, which are ubiquitous in most carbonate rock types. However, stylolites can also develop in other rock types such as sandstones, shales or evaporites (Young, 1945; Heald, 1955; Wright and Platt, 1982; Rutter, 1983).

Stylolites are important because (1) they are indicative of the amount of chemical compaction or shortening that a rock has experienced (at the stylolite, Rispoli, 1981; Petit and Mattauer, 1995); (2) they can be used to calculate overburden or tectonic stress (Schmittbuhl et al., 2004; Renard et al., 2004; Koehn et al., 2007, 2012; Ebner et al., 2009a, 2010a; Laronne Ben-Itzhak et al., 2012) and (3) they may constitute fluid-flow pathways or barriers and thus affect the permeability distribution of the host rock (Carozzi and von Bergen, 1987; Alsharhan and Sadd, 2000). Chemical compaction here refers to the dissolution at the stylolite interface, and concomitant material precipitation in pores or transport out of the system, that leads to overall compaction. On the outcrop scale, stylolites are planes that collect relatively insoluble material during dissolution that has different properties than the host rock so that the overall rock becomes anisotropic. The simplest example for this anisotropy is the tendency of stylolite-bearing rocks to break along stylolite planes (Baud et al., in press). This weakness of the stylolite plane and its tendency to fracture may be enough to enhance fluid flow along the stylolite plane. In addition, accumulation of materials, such as clays, on the stylolite plane may reduce the permeability perpendicular to the stylolite plane (Dunnington, 1967; Nelson, 1981; Koepnick, 1987; Finkel and Wilkinson, 1990; Dutton and Willis, 1998; Alsharhan and Sadd, 2000), although the flanks of teeth may be areas of increased permeability (Carozzi and von Bergen, 1987; Dawson, 1988; Raynaud and Carrio-Schaffhauser, 1992; Van Geet et al., 2000; Gingras et al., 2002; Harris, 2006).

Other studies found no effect of stylolites on a rock's overall permeability (Lind et al., 1994; Heap et al., 2014).

Stylolites are dynamic interfaces with self-affine properties. They are typically rough on the small scale and flat on the large scale (Renard et al., 2004, Schmittbuhl et al., 2004, Ebner et al., 2009, Rolland et al., 2012, 2014). The growth of the roughness is triggered by heterogeneities in the rock, for example impurities that affect dissolution, the grain size distribution or the solubility of different components. Recent research based on analytical and numerical analysis suggests that these heterogeneities may trigger localized dissolution (for example through a chemical effect) and thus lead to the development of the stylolite plane in the first place (Aharonov and Katsman, 2009). The noise that pins the interface (Ebner et al., 2010b) leads to preferred dissolution at mainly one side of the stylolite and thus produces the growth of teeth (Koehn et al., 2007). Surface and elastic energies counteract the development of roughness in favor of a flat surface. Surface energy dominates on the small scale (μm) and the stylolite surfaces at this scale are relatively rounded, whereas elastic energy takes over on the large scale (typically several μm to mm) where the stylolites become first rough (Schmittbuhl et al., 2004; Koehn et al., 2012) with pronounced teeth or spikes and then on the m- to tens of m-scale flat again. This scale transition also happens through time. The stylolite roughness initially grows very slowly in the surface-energy dominated, non-linear regime (unless the grain size is very large) with a growth exponent of about 0.5 (Ebner et al. 2009b). Once the growing wavelength of the stylolite has reached a critical scale, the amplitudes start to grow in the elastic energy dominated regime where the roughness grows faster (growth exponent around 0.7 to 0.8; Koehn et al., 2007). Although Koehn et al. (2007) proposed that the growth law can be used to estimate the amount of compaction at a stylolite, the estimate is not very precise, owing to its non-linearity and the fact that the parameters are based on numerical simulations only. However, if a larger object (such as a grain or fossil) pins the stylolite surface, the growth becomes linear and the full stylolite compaction can be determined (Koehn et al., 2012). The following question arises: how to identify the growth dynamics of a specific stylolite in order to be able to estimate its compaction?

Several classifications of stylolite shapes exist (e.g. Park and Schot, 1968; Alsharhan and Sadd, 2000; Vandeginste and John, 2013). The classification of Park and Schot (1968), which is also used by Vandeginste and John (2013) uses up to six different shapes (rectangular up and down, seismograph, wavy, sutured, sharp-peak). It is, however, not always easy to apply and is not consistent with an understanding of the dynamics of stylolite evolution. Alsharhan and Sadd (2000) use a much simpler classification (rectangular or high-amplitude; solution seams or wave-like; wispy seams or horse-tail), which also incorporates the connectivity of stylolite networks. However, this classification is very general and does not include realistic compaction estimates, because the authors do not separate linear from non-linear amplitude growth (Koehn et al., 2012). Ignoring this may lead to significant underestimates of the actual chemical compaction at a stylolite. A more sophisticated stylolite classification is needed to achieve realistic estimates of chemical compaction and

sealing in stylolite-dominated rocks. Using a variety of stylolites from Zechstein cores from a lean gas field in northern Germany in combination with a large collection of stylolites from a range of field areas around the world, as well as a series of numerical simulations, we present a new classification of stylolites that is coherent with their formation, that allows the separation of non-linear from linear growth and that can be used to estimate the stylolite's influence on rock permeability.

2 Natural examples

We studied six reservoir cores of the Zechstein 2 carbonates unit (Ca₂), also called Stassfurt carbonate, located at the southern margin of the southern Permian Zechstein basin (Ziegler, 1990; Taylor, 1990). The cores are provided by ExxonMobil Production Germany and their exact location is not provided here due to confidentiality. One of the cores is from 3720 to 3750 m below surface and the other five from 3950 to 4050 m approximately. The Ca₂ sediments were deposited on paleosurfaces of the Werra Anhydrite and are sealed by the overlying basal Anhydrite (Sannemann et al., 1978). They represent slope deposits (Strohmenger et al., 1996) and form an important lean gas reservoir. After the initial sedimentation in the Permian these deposits were subject to fast subsidence in the Mid Triassic (down to 2500m), slow subsidence at the beginning of the Cretaceous (down to 3800m), fast subsidence in the Mid Cretaceous reaching the maximum burial depth (at about 4700m) and an uplift event at the end of the Cretaceous up to 3750-4000m followed by only minor events up to date (Bruns et al., 2013). The original limestone units with an initial porosity of up to 42% (Bruns et al., 2013) have been first dolomitized and later on calcitized (dedolomitized) and there is evidence for several phases of fracturing and fluid fluxes that partly resulted in leaching and fracture healing (by formation of veins and precipitation of ore minerals, for example Galena). The studied cores contain abundant sedimentary stylolites of various shapes and a smaller number of tectonic stylolites. The amplitude of the sedimentary stylolites varies by more than an order of magnitude, ranging from small mm-amplitude stylolites to those having teeth longer than 40mm. Most of the high-amplitude stylolites enclose a large amount of dark material at the teeth (fig. 1a,c; rectangular after the classification of Parks and Schot, 1968), whereas the small stylolites show roughness on several scales (fig. 1c, sutured or sharp peaked after Parks and Schot, 1968) with some having larger amplitudes. We studied stylolites in two cores in detail (table 1) where we count the amount of stylolites per meter core and use the amplitude of the stylolites to estimate the chemical compaction. A conservative estimate of the compaction uses the sum of the maximum amplitudes of all stylolites as vertical dissolution and relates this number to the studied core length. The results show a relatively low effect of stylolites that only account for 3 to 5.6 percent of compaction of the cores. However, if we use a new calculation method that is explained in the discussion section of this contribution, the chemical compaction at the stylolites can be estimated to be in the order of 25 to 39 percent, almost one order of magnitude larger than the conservative estimate.

Several factors indicate that the stylolites do influence fluid fluxes (fig. 2). Dissolution holes that are located at stylolite teeth are likely produced by leaching fluids (fig. 2a). In this case the stylolite may form local barriers for fluid

flow so that the fluids remain longer below teeth and thus have time to produce the holes. The second indicator are veins that are often found on the flanks of stylolite teeth (fig. 2b). This indicates that the flanks of teeth are potentially dilatant sites that are used as fluid pathways. The stylolites also influence at least the late stage calcitization (de-dolomitization, fig. 2c,d), where the stylolite itself seems to protect the dolomitized phase and both sides of the stylolite show different amounts of calcitization. A late stage hydrothermal fluid in the Zechstein cores leads to the precipitation of Galena in fractures. Figure 3 shows a stylolite with pronounced teeth and a relatively thick seam. The Galena precipitates below the stylolite seam (fig. 3b) and can only infiltrate the first part of the seam (fig. 3c). Along the teeth flanks Galena precipitates in cracks and can be found all along the flanks (fig. 3d). Away from the teeth no Galena can be found next to the stylolite seams (fig. 3e). We argue that the Galena is a tracer for differential fluid flux across this stylolite, fluids travel along the teeth flanks and are locally stopped by the stylolite seam that acts as a barrier. In summary, the stylolites show evidence of a pronounced influence on reactions and fluid fluxes through the Stassfurt carbonate at least on the local (stylolite) scale.

3 Numerical Model

We use the software “ELLE – Latte” (Koehn et al., 2003; Bons et al. 2008) for the presented simulations with a similar setup to the work of Koehn et al. (2006, 2007, 2012) and Ebner et al. (2009b). The model is two-dimensional with dissolution triggered at an initially flat interface and studies the roughness evolution of stylolites. In this contribution we expand the model from previous work to include stylolites that nucleate and grow in a rock that has layers, which dissolve with variable dissolution rates. We then compare the growth of layer dominated stylolites with previous studies of uniform and bimodal stylolite growth in order to derive a classification of stylolite shapes that can be used for quantitative calculations. As was discussed in the introduction the roughening of stylolites is initiated by pinning material in the hostrock, otherwise elastic and surface energies as well as normal stress gradients will keep the surface flat. An example of these flat interfaces in rocks are dissolution cleavages, where the roughening component is missing. Sedimentary layer boundaries as such are stable and remain flat during dissolution unless the layers contain additional smaller scale heterogeneities. In the model we initiate layer dissolution within a layer and not at the boundary. Compression in the model is vertical with displacement-controlled deformation assuming a sedimentary overload and the left- and right-hand boundaries are friction free (fig. 4). The solid (the stressed rock) is described by a lattice spring model where circular particles of a uniform size are connected to each other by six linear elastic springs that experience normal and shear forces (fig. 4; Sachau and Koehn, 2014). The model lattice is triangular with horizontal rows of particles where each second row is offset. The springs are used to calculate the local stress field at a particle and its elastic energy E_{el} from the strain tensor u_{ik} according to (Landau and Lifshitz, 1986)

$$E_{el} = \frac{1}{2} \lambda_1 (\sum_i u_{ii})^2 + \lambda_2 \sum_{i,k} u_{ik}^2, \quad eq. 1$$

where λ_1 and λ_2 are the Lamé constants. Particles that are not connected by springs (for example those at the stylolite interface) experience repulsive forces

once they come into contact. Particles along the stylolite interface have a surface energy. The surface energy E_s of an interface particle is calculated by an average of the curvature ρ of the interface (Koehn et al., 2007) according to

$$E_s = \gamma \frac{1}{\rho}, \quad eq. 2$$

with γ being the interfacial free energy between fluid and solid. For the interface dissolution it is assumed that transport of material is instantaneous and that the pore space is large enough for material to precipitate. Dissolution of particles at the interface is a function of the difference in elastic energy between a stressed and a non-stressed solid, differences in surface energy between a flat and a curved interface (with a convex interface driving dissolution and a concave interface driving precipitation) and differences in normal stress along the whole interface assuming that the fluid has an average saturation. Each particle has a given mass, which is used to calculate which particle dissolves fastest during a time step. Only the fastest-dissolving particle is taken out of the model, the solid is relaxed and the next particle can dissolve. A linear rate law with a given rate constant is used to calculate the dissolution rate D_i according to

$$D_i = k_i V_s \left(1 - \exp \frac{-\Delta\sigma_n V_s - \Delta E_s - \Delta E_{el}}{RT} \right), \quad eq. 3$$

with k_i being the dissolution rate constant of the particle i , V_s the molecular volume of the solid, R the universal gas constant, T the temperature, and σ_n the normal stress across the interface (Koehn et al., 2003; 2007; 2012). There are several assumptions in this model. The aim of the modeling is to study the roughness evolution of a single stylolite, so that the initial dissolution does start at a given flat interface. In a real rock this localization of dissolution could happen at the boundary of a sedimentary layer or at several horizontally aligned clay particles in a rock. The kinetics of the model are dissolution limited because transport and precipitation of material are not included. This means that the model has no “real” time scale. However, we argue that the roughness evolution is a function of the compaction of the rock as long as material can precipitate in pores or is taken away and the stylolite has enough time to grow (Koehn et al., 2007; 2012). We also note that equation 3 contains difference in normal stress as well as differences in elastic and surface energy. In the presented model the difference in normal stress across the interface is given as the difference between the normal stress at a given particle and the mean normal stress of the whole interface. This approach assumes that the fluid is saturated with respect to the stressed solid. It turns out that with this approach the magnitudes of the normal stress difference and the Helmholtz free energy difference (elastic and surface energy) are of the same order. Koehn et al. (2007; 2012) compared the scaling of this modeling approach with an analytical solution and data from natural stylolites and found that the natural scaling can only be reproduced if this approach is taken.

The final input into the model is the representation of heterogeneities in the rock (quenched noise). Heterogeneities in the model are described by a variation of the dissolution constant in equation 3. A variation of this parameter will typically represent different minerals or grains in the original rock. Quenched noise is

added to the system in three different ways. The smallest noise is set on the particles themselves, so that a given number of particles in the model has a dissolution constant that is a factor x smaller than the overall dissolution constant. This variation can be represented of different minerals in the original rock. A larger-scale noise can be put on “grains” that are inherited from the initial microstructure, where grains consist of a given cluster of particles that have a different dissolution constant than other grains (Koehn et al., 2012). Lastly, whole horizontal layers (for example bedding in a real rock) can have different dissolution constants relative to the rest of the model. We generally apply at least two noises, having a small-scale noise in addition to either larger-scale grains or layers. Noises are overlapping, so that, for example, the grains themselves also contain a smaller scale noise (fig. 4). Noise is essential for roughening as the system does not develop stylolites without noise.

4 Results

We performed about 100 simulations with mainly layer-dominated stylolite growth. All simulations have a lattice size of 200 particles in the x-dimension (overall lattice has 46,000 particles), last for 30,000 time steps and start with a row of particles taken out in the middle of the model. Parameters of the simulations are: dissolution constant for calcite is $0.0001 \text{ mol}/(\text{m}^2\text{s})$, the molar volume for calcite is $0.00004 \text{ m}^3/\text{mol}$, the temperature is 500 K, the surface free energy is $0.27 \text{ J}/\text{m}^2$, the Poisson ratio is 0.33, the Young’s modulus is 40 GPa and the real physical width of the system is 10 mm (Koehn et al., 2007; 2012). These parameters represent dissolution of an average limestone at the given temperature and it’s elastic properties, only the Poisson ratio is dictated by the model setup.

4.1 Normal roughening and grain pinning

Normal roughening of stylolites and grain pinning has been discussed in detail in Koehn et al. (2007, 2012) and Ebner et al. (2009b). By pinning we mean that a slower-dissolving particle or particle cluster sits on one side of the interface so that only the other side dissolves. This leads to a relative movement of the pinning point away from the average interface. In our models we push from the upper and lower boundary, so that the average interface remains in the middle of the model. Teeth then grow downwards if pinning particles come from above the interface and they grow upwards if pinning particles meet the interface from below. We give one example of grain pinning and small-scale roughening in order to discuss the differences and similarities with the layer-dominated growth. In this example the background noise on particles is set such that 10% of particles dissolve at a velocity of 80% of the matrix and 5% of the larger grains also dissolve slower (fig. 5). The roughening behavior of the interface changes completely from small-scale roughening, with only small pinning particles meeting the interface, to larger-scale roughening when a large pinning grain enters the stylolite. Small-scale roughening can be seen on the right hand side in the simulation of figure 5, where no larger grain meets the interface. The growth of the roughness amplitude is very low, because pinning is happening from both sides of the interface so that pinning particles meet each other, and elastic and surface energies are also high enough to dissolve single pinning particles. The amplitude of the stylolite on the right hand side does not resemble the

dissolution that has happened at the interface. Amplitude growth is strongly non-linear and chemical compaction estimates would be underestimated significantly. On the left hand side larger-grain pinning dominates the stylolite. The length of a tooth depends on the time when the grain reaches the stylolite and how fast the grain itself is dissolving. The tooth on the very left hand side shows almost the full dissolution that is happening at the interface from one side, because the grain met the interface early on and is still pinning. Note however, that a tooth growing from the median plane of the stylolite can only capture half of the dissolution. In order to get the full chemical compaction one has to either measure the distance from a downwards tooth to an upwards tooth or use the distance between median surface and the largest tooth and multiply by two.

4.2 Layer pinning

In order to simulate the growth of layer-induced stylolites that we find in the Zechstein cores, we insert an initially horizontal layer in the model. Its thickness is 6% of the overall box thickness so that the layer is 0.6 mm thick in real space. Noise in the matrix is set such that 10% of particles dissolve slower by an amount of 80% to 99.9% of the matrix dissolution. The layer itself contains the same particle noise plus all particles of the layer dissolve 56% to 80% slower than the matrix. The stylolite starts within the slower dissolving layer (fig. 6). Due to the lattice configuration the initial interface is not positioned exactly in the middle, but is just above the middle. This means that the stylolite has to dissolve a little bit less of the layer on the upper side. The initial roughening is triggered by the particle noise in the layer and a small wavelength develops while the layer is being dissolved. At some point of increasing wave amplitude, the dissolution surface reaches the matrix either above the layer (at stylolite peaks) or below the layer (at stylolite troughs). A peak means that parts of the layer are still present below the stylolite and a trough means that parts of the layer are still present above the stylolite. Because the initial stylolite seed was not exactly in the middle of the layer the stylolite reaches the upper edge of the layer earlier and has more layer below than above itself. This initial roughening stage is very slow, the amplitude growth is non-linear and dissolution will be underestimated if the amplitude height is used as a compaction estimate. We term this initial roughening stage nucleation. The duration of this nucleation stage will change with the thickness of the layer.

Once the stylolite has reached the edge of the layer, the layer is pinning the interface because it dissolves slower than the matrix. This means that all the teeth that reach the matrix above the stylolite will grow relatively upwards and all teeth that reach the matrix below the stylolite will grow downwards. Now the stylolite is recording the full compaction and the growth of teeth is linear and “fast”. The width of the teeth is a function of the initial roughening of the stylolite in the layer and varies from single pinning particles to the largest wavelength that the roughening achieved during the nucleation stage, in our simulations up to about 1/5th of the width of the simulation (2mm). The width is restricted by the system size (in our case the 200 particle-wide box), so that real systems with a much larger size can develop wider teeth (fig. 1). The roughness of the teeth themselves depends on the initial particle noise in the system. The teeth are only flat in the simulations if this initial noise is very low (10% of particles dissolve with a dissolution of 99% to 99.9% of the matrix). This suggests that the stylolite

in figure 1a grows in a rock that does not have much noise on the small scale (few heterogeneities). Pinning of the stylolite produces the typical rectangular stylolites of Park and Schot (1968) with residual material at the teeth. Rectangular upwards has residue below the teeth and rectangular downwards has residue above the teeth. Whether or not a stylolite is dominated by one or the other (upwards or downwards) depends on its initial position relative to the layer.

Once a stylolite reaches the stage where the layer is pinning the interface, the teeth record the chemical compaction history in a linear way and they can become very long (fig. 1b). However, the pinning layer may also dissolve, even if its dissolution is much slower than that of the matrix. This means that the stylolite will start to lose its pinning capabilities (fig. 7). Once the layer is gone the stylolite becomes almost stationary with only small changes at the corner of teeth making it rounder (fig. 7a,b). The roughness growth that is triggered by the background noise (on the particle scale) is very slow and non-linear and cannot change the large amplitude that was produced by the pinning layer. The stylolite has an unusual shape and only records part of the compaction history (fig. 1b may be an example, large amplitude stylolite).

We separate the growth of layer-dominated stylolites into three stages (fig. 8): stage I represents the nucleation stage where the stylolite roughens within the layer, stage II is the pinning stage when the stylolite records the chemical compaction in a linear way growing fast and stage III is only reached once the layer is fully dissolved and the stylolite becomes stationary. The transition between stages II and III depends on how easily the pinning layer is dissolved. In the four cases shown in the graph of figure 8, numbers represent the factor by which the layer dissolves slower than the matrix. At 60% and 62% the layer dissolution is too slow and the stylolites continue growing their teeth and pinning. At 64% the layer dissolves slowly so that only part of the compaction history is recorded. At 68% the layer dissolves fast and the teeth only record about 1/6th of the compaction history. We illustrate the transition between pinning and dissolving layers in the simulations in a graph of matrix noise (noise on the particle scale) versus layer noise (fig. 9). The graph shows that the layer has to dissolve slower if the matrix noise is low in order for the layer to pin, whereas with a higher background noise the layer dissolution can be less in order for it to pin. The relation is non-linear and indicates that the layer cannot pin if there is no matrix or particle scale noise. A transition zone exists where the layer is partly dissolved but still has some pinning teeth. This produces shapes that are similar to the “seismogram” type of Park and Schot (1968), with a median surface that produces “normal” non-linear background roughening and some pronounced teeth. The roughness in these stylolites is developing on two very different scales or amplitudes (fig. 10). This shape is also similar to stylolites that grow in a rock with bi-modal noise, with a particle noise and a noise on the larger scale, for example large grains (fig. 5) or fossils.

5 Discussion

5.1 Classification

Based on our simulations and observations of stylolites in the Zechstein Ca2 cores as well as observations of a large collection of stylolites from a range of field areas around the world, we present a new classification of stylolite shapes

(fig. 11, 12). This classification refines the original one by Park and Schot (1968), proposing only 4 types of stylolites: (1) rectangular layer, (2) seismogram pinning, (3) suture/sharp peak and (4) simple wave-like. Rectangular layer stylolites (type 1) is a sensible class without the addition of facing up or downwards. Up or downwards facing varies even within a single stylolite and has no significant meaning. The addition of the term “layer” to the classification of rectangular stylolites is important, because some rectangular-looking stylolites can also develop from normal roughening, and they have different properties than the typical layer dominated ones. Seismogram pinning (type 2) implies that the stylolite experiences noise on several very different scales and this is important for compaction estimates. A seismogram pinning stylolite in our classification typically has a median surface with small-scale roughening and one or several large teeth with a pinning source. The rectangular and seismogram pinning stylolite types were merged in a single class by Alsharhan and Sadd (2000). Suture and sharp peak (type 3) stylolites should represent one single class, because it is not clear when a stylolite is sutured and when it is sharp peaked. In the simulations the shapes can result from the same noise and hence differentiating them is not useful. This class would incorporate normal growing stylolites (with only small scale noise) as well as layer-growth stylolites where the layer is gone. The latter are hard to distinguish from normal roughening stylolites, and therefore they are both included in one single class. The final type (4) are the simple wave-like stylolites, which are not very common in the Zechstein cores (less than 2% of stylolites) but are frequent in many other carbonate areas. The first two classes, rectangular layer and seismogram pinning typically show signs of pinning grains, fossils or layers. The last two types, suture/sharp peak and simple wave-like do not show evidence of larger scale pinning structures and only sometimes develop straight teeth.

5.2 Compaction

The advantage of our stylolite classification is that it can be directly used for compaction estimates. Rectangular layer stylolites pin best and grow linearly as a function of chemical compaction along the stylolite. They can be used to get a realistic chemical compaction estimate for rocks (for the stylolite compaction) and may be representative for dissolution on the other stylolites as well (i.e. those that belong to the other types). Compaction may still be underestimated even when type (1) stylolites are used, because their nucleation stage involves non-linear growth (however, this initial growth stage may be minor). The second class, seismogram pinning type stylolites, typically have a bi-modal roughness. Similar to rectangular stylolites the pinning teeth may represent most of the actual compaction. This is especially true if the teeth contain remnants of layers. If the teeth represent fossils or grain pinning, then only part of the compaction is recorded, from the moment the fossil or grain meets the stylolite up to when compaction stops. In these cases the longest teeth give the most reliable estimates of the minimal compaction. Seismogram pinning stylolites often have a median surface. If this surface can be identified, then only one tooth is enough to measure compaction. The amount of compaction on the stylolite is at least two times the distance between the tooth tip and the median surface. The longest tooth will always be the most reliable estimate. The last two classes of stylolites are less suitable for compaction estimates. Class 3, normal suture and sharp peak

type stylolites grow non-linearly. Therefore a simple measurement of the roughness amplitude is not representative for the amount of dissolution on the stylolite (Koehn et al., 2007; 2012). However, the compaction A can still be estimated using the scaling law of Koehn et al. (2007) and Ebner et al. (2009b):

$$A = x \left(\frac{w}{l} \right)^{\frac{1}{\beta}} l, \quad eq. 4$$

where l is the grain size, β a growth exponent (0.5 in the small scale regime and up to 0.8 in the large scale regime), x a compaction pre-factor that has a value of around 15 in simulations of Ebner et al. (2009b) and w the mean width of the interface according to

$$w_{(L)} = \sqrt{\frac{1}{L} \sum_{i=1}^L [h(i) - \bar{h}]^2}, \quad eq. 5$$

with L being the number of points measured along the stylolite, h the height of point i and \bar{h} the average height of the interface (larger amplitude stylolites have a higher mean width). For example in the Zechstein, a small stylolite with a mean width of 1mm, a grain size of 0.01mm and a growth exponent of 0.8 does represent 4 to 5cm of local chemical compaction. In the Zechstein cores this compaction estimate on a small suture or sharp peak stylolite then gives the same order of compaction as the rectangular layer types (up to 4cm). This may mean that all stylolites have experienced a similar chemical compaction. We studied two Zechstein cores in detail (table 1) and measured 2754 stylolites. The vertical compaction or dissolution of the core as a function of stylolites gives a value of 3.01 to 5.62% in the case where only the maximum tooth height of every stylolite is taken into account (with an average of 4.32% for both cores). These values are most probably a strongly underestimated. If we use all tracking stylolites in these cores (only 2% of stylolites) that belong to type 1 or 2, we derive at a mean linear dissolution of 1.43cm at these stylolites. Assuming that the other non-linearly growing stylolites show a similar dissolution, the compaction estimates are 25.43 and 39.15% for the two cores (with an average of 34.04% for both cores). If one compares the chemical compaction estimate at stylolites with the initial porosity estimates of the Zechstein carbonates of up to 42% (Bruns et al., 2013), these values indicate that dissolution at stylolites is the dominant compaction process in these rocks. In addition these values indicate that material that dissolves at stylolites does not have to leave the system but can fill pore space. However, more tests are needed in order to improve reliability of these estimates. Simple wave-like stylolites are the worst for compaction estimates, because they may represent dissolution seams that have not seen much chemical compaction or they grow highly non-linear with a very low growth exponent and are therefore very unreliable.

5.3 Barriers and leaks

Our classification can also help for assessing the anisotropy of permeability across different stylolites. Figures 2 and 3 illustrate that the stylolites in the Zechstein do influence fluid flow locally. The most important ingredient is the collection of sealing material in the stylolite. If the material is not sealing (as was

the case in the study of Heap et al., 2014) the stylolites or part of them cannot be local barriers to fluid flow. In general stylolites can perform three different structural changes to produce barriers: (i) they can collect impermeable material and thus build up a barrier, (ii) they can intensify the existing sealing properties of layers and (iii) they can offset existing barriers (fig. 11). Collecting material and intensifying dissolution creates barriers whereas offsetting destroys barriers. Rectangular layer (type 1) stylolites are characterized by an intensification of barriers at the tips of the teeth and an offsetting of initial layering creating new pathways for fluids across the flanks of teeth. This class of stylolites creates very anisotropic permeabilities (fig. 3) and can potentially destroy seals. The behavior of the seismograph pinning type (2) is more complicated. As long as layers pin at the teeth the structuring is similar to the rectangular layer type. However, the structuring of the median surface depends on how much material can be collected in the stylolites and what properties that material has. If the material is sealing and the median surface is not very rough, then it can develop into a barrier that is only breached at the existing larger teeth. Suture and sharp peak type (3) generally collect material. In this case they may create barriers, especially if they do not become very rough and if the collected material is sealing. Local spikes may still breach the barriers (for example see Koehn et al., 2012, figure 1b). Simple wave-like stylolites (type 4) may represent dissolution seams, quite often contain insoluble material and can represent original sedimentary layers or other sedimentary or diagenetic surfaces. This class can build good barriers, because the stylolites are not rough and are thus not offsetting the barrier.

A quantitative indicator for stylolite permeability or sealing quality could be the measure of sealing versus non-sealing material along the stylolite. This implies, however, knowledge of the sealing qualities of different parts of the stylolite. In addition a three-dimensional morphology analysis would be ideal. If we perform a two-dimensional analysis of the stylolites shown in figure 1a and b, stylolite 1b has a sealing capability of only 15%, whereas stylolite 1a has a local sealing capability of around 75%. Further research is needed in this direction in order to quantify sealing qualities and local versus larger-scale permeabilities of these complex structures following the work of Heap et al. (2014).

6 Conclusion

Our study shows that stylolites in the Zechstein 2 carbonate units can influence reactions and fluid flux and can be used to estimate compaction. Stylolites typically have three different end-members of noise: background noise on the small-scale (small grains or secondary phases), noise on the larger-scale (large grains or fossils) and noise in the form of sedimentary layers. How these different noises interact and which noise is dominant determines which class of stylolites form. We present a new classification of stylolites based on our simulations, observations of natural stylolites and a variation of the original classification of Parks and Schot (1968). Our proposed advanced classification separates stylolites into 4 classes: 1) rectangular layer type, 2) seismograph pinning type, 3) suture or sharp peak type and 4) simple wave type (fig. 12). Rectangular layer type stylolites develop at layer interfaces, grow linearly, are the best indicators for the actual amount of chemical compaction at stylolites and are offsetting and thus destroying local seals. They typically have a highly

variable local permeability with barriers at the tips of teeth and leaks at the teeth flanks. Seismogram pinning type stylolites often contain remnants of layers or pinning grains, typically have a median surface, and their largest teeth can grow linearly so that these teeth can be used for compaction estimates. Their effects on permeability are complicated, since large teeth can offset and destroy original seals but the median surface may also collect sealing material. Suture or sharp peak type stylolites are the most common and can have variable shapes, they develop mainly as a function of a relatively uniform noise without large pinning grains or layers, and they grow very non-linearly so are thus not very accurate for the use of compaction estimates. This class of stylolites can potentially create barriers if they collect enough sealing material during their growth and if local spikes do not breach the barrier. Stylolites of the last class, simple wave-like types, do not show a large roughness and often contain original layer material, so they can be good seals. They are, however, very hard to use for compaction estimates and may not represent a lot of local dissolution.

7 Acknowledgements

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Figures

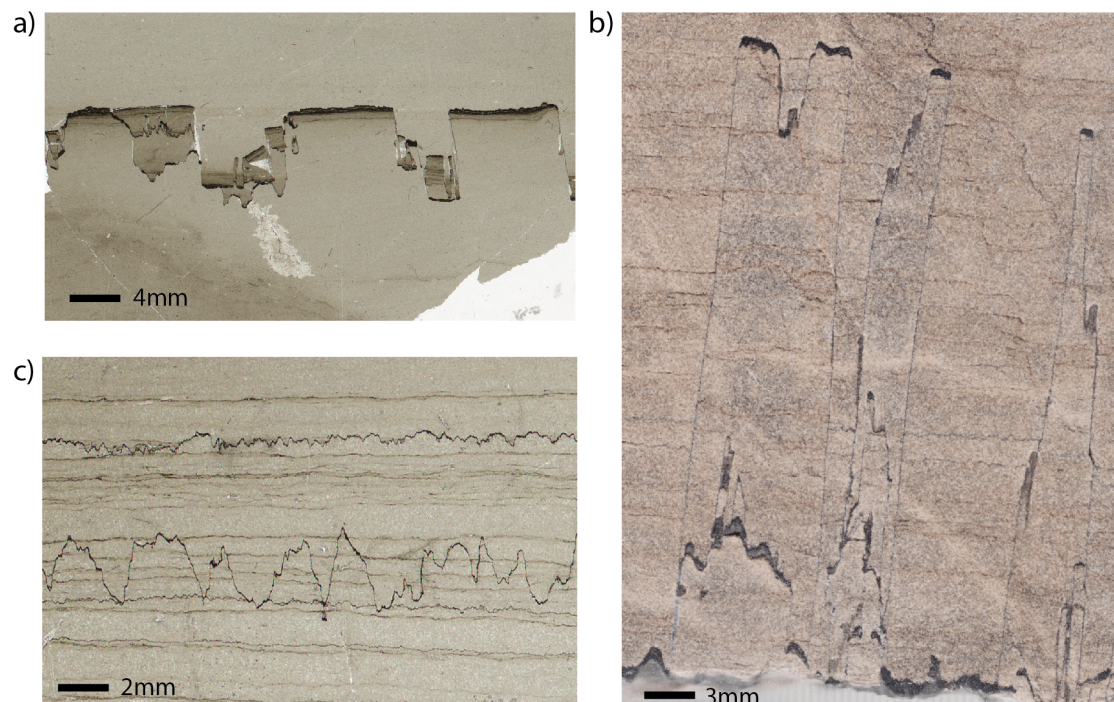


Figure 1 Examples of variable stylolite shapes from the Zechstein cores. a) different roughness amplitude stylolite with a self-affine roughness and multiple wavelengths. b) extremely long teeth with remnants of sedimentary layers on the tip of teeth. Teeth have very straight flanks. c) rectangular stylolite with remnants of layers at stylolite teeth tips. Some veins are visible at teeth flanks.

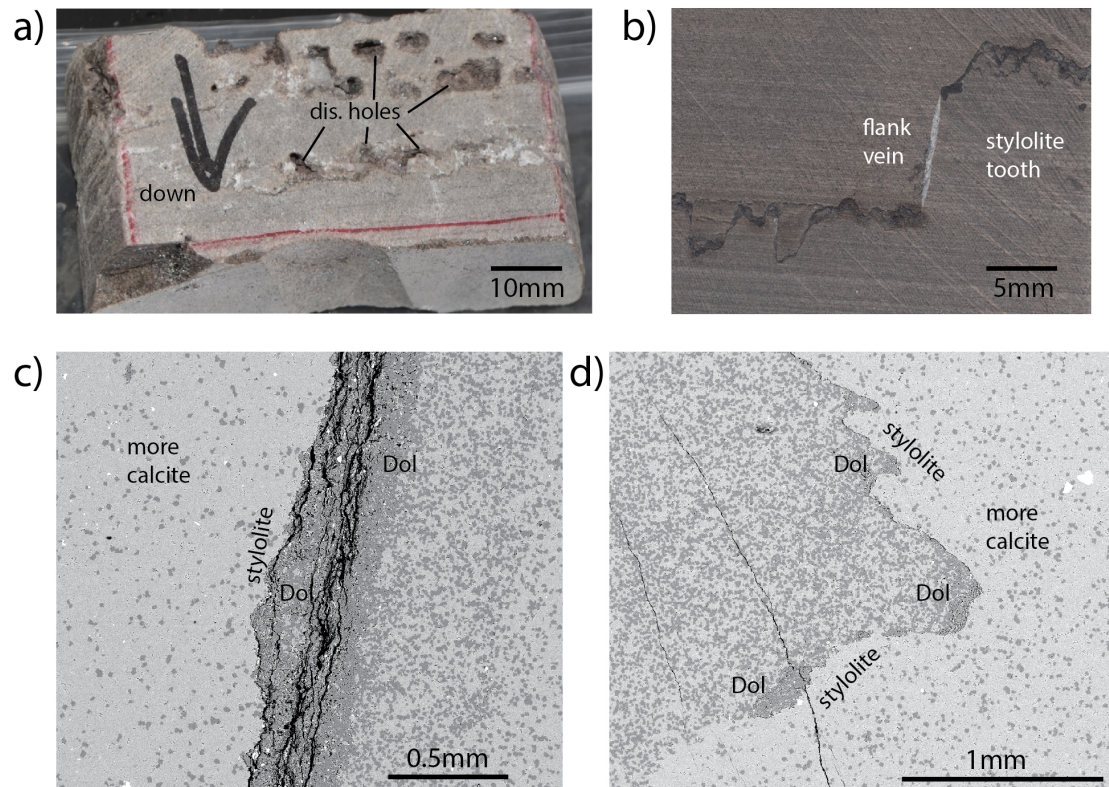


Figure 2 Stylolites influence fluid flux and reactions. a) dissolution holes at stylolite teeth (arrow points core downwards). b) vein at tooth flank indicating potential fluid flux across teeth, c) SEM picture with light grey representing calcite and darker grey dolomite (plus the stylolite itself in black). Recrystallization is different on both sides of the stylolite. d) another example with the same settings as c, where the calcitization (de-dolomitization) changes across the stylolite.

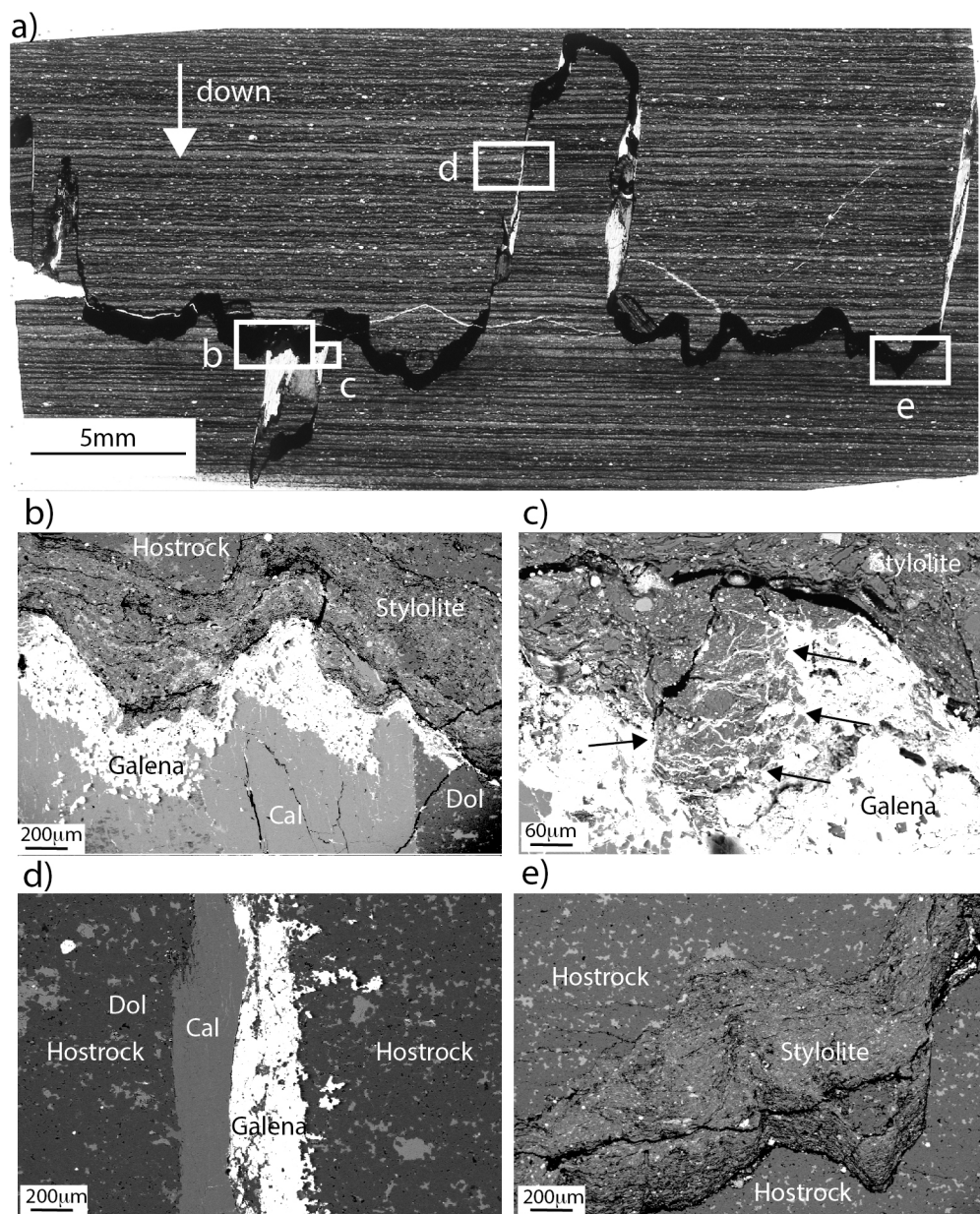


Figure 3 Precipitation of Galena in a stylolite from the Zechstein cores. a) shows an overview of the stylolite with pronounced teeth and thick dissolution seams. b) below the seams at the end of a tooth flank Galena precipitates indicating that the fluids cannot breach the stylolite and that the stylolite forms a local barrier. c) detailed view of b) showing how the Galena rich fluids infiltrate the sealing material but cannot breach it. d) tooth flank with precipitation of Galena indicating that the fluids travel along teeth and the stylolite leaks at the flanks of teeth. e) close up of the stylolite seam with no Galena. Cal is calcite and Dol Dolomite.

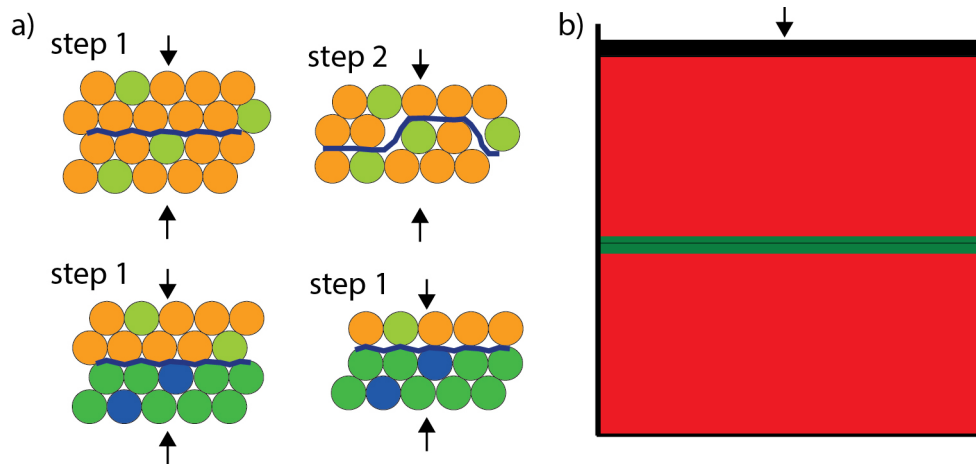


Figure 4 a) sketch of part of the numerical lattice (round discs) with the initial stylolite interface (blue line). Particles have different dissolution constants, with the light green particles representing those that dissolve slower. The upper setup produce small scale roughening and complex dissolution of either particle below or above the interface depending on their dissolution constants. The lower model shows an added layer where all the particles below the stylolite belong to a layer that dissolves slower. Blue particles represent smaller noise in the layer, these dissolve even slower than the rest of the layer. The layer “pins” the interface so that all particles above the stylolite dissolve. b) shows model setup with the layer in the center (in green). The stylolite starts within the layer.

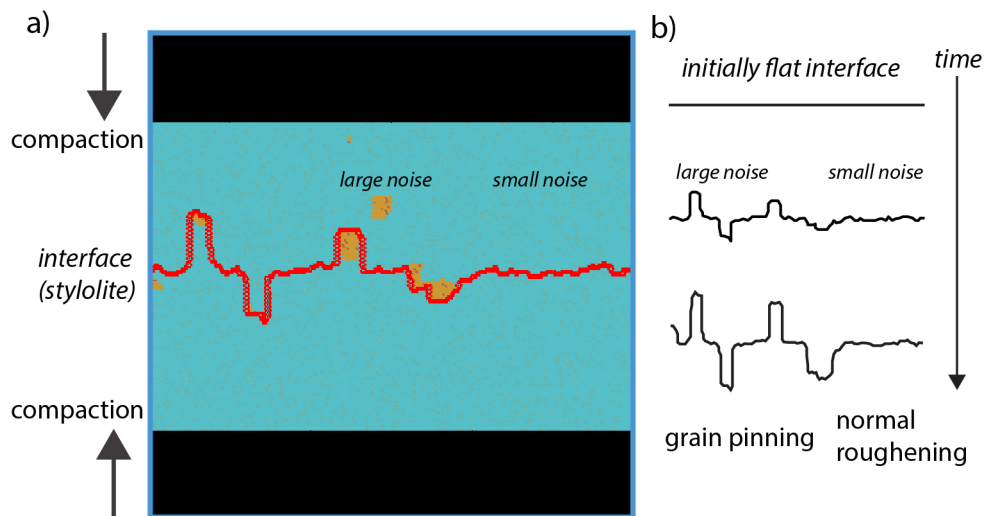


Figure 5 a) Simulation run with stylolite in red, lost material of the original box in black (displacement on upper and lower boundary), background material in blue and slower dissolving small and larger scale noise in orange. b) shows a time series of the simulation from an initially flat interface. Normal small scale roughening develops on the right hand side with very slow amplitude growth, so that the surface is just fluctuating. Larger grains are pinning on the left hand side as soon as they meet the interface and record the compaction in a linear way once they are pinning. The large tooth on the left hand side records half of the dissolution on the stylolite (illustrating that teeth that grow from the median surface always represent only half the dissolution).

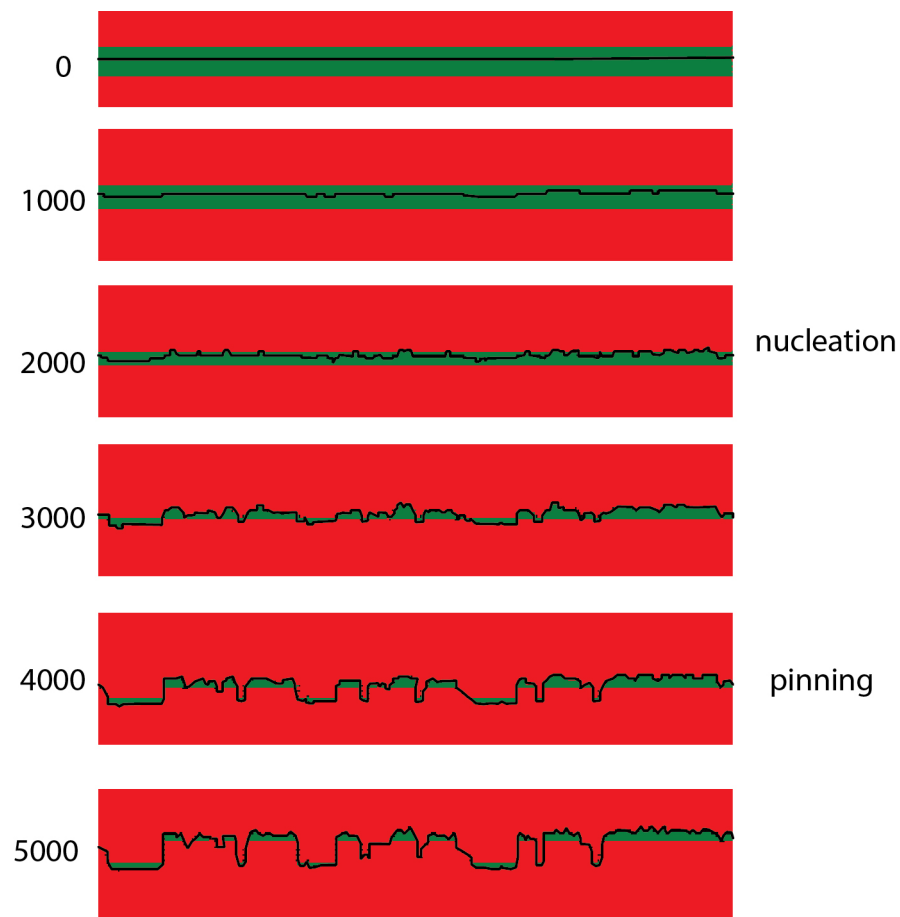


Figure 6 Illustration of the layer pinning. Initially the stylolite starts within the layer and roughens (the layer also needs to be heterogeneous; nucleation stage). Once the stylolite breaches the layer on one side the layer starts to pin. The slower dissolving material is located at the growing side of the teeth (top of teeth if growing upwards, bottom of teeth if growing downwards). Once the layer pins the growth is linear with respect to the boundary displacement and the teeth track the full compaction of the model system.

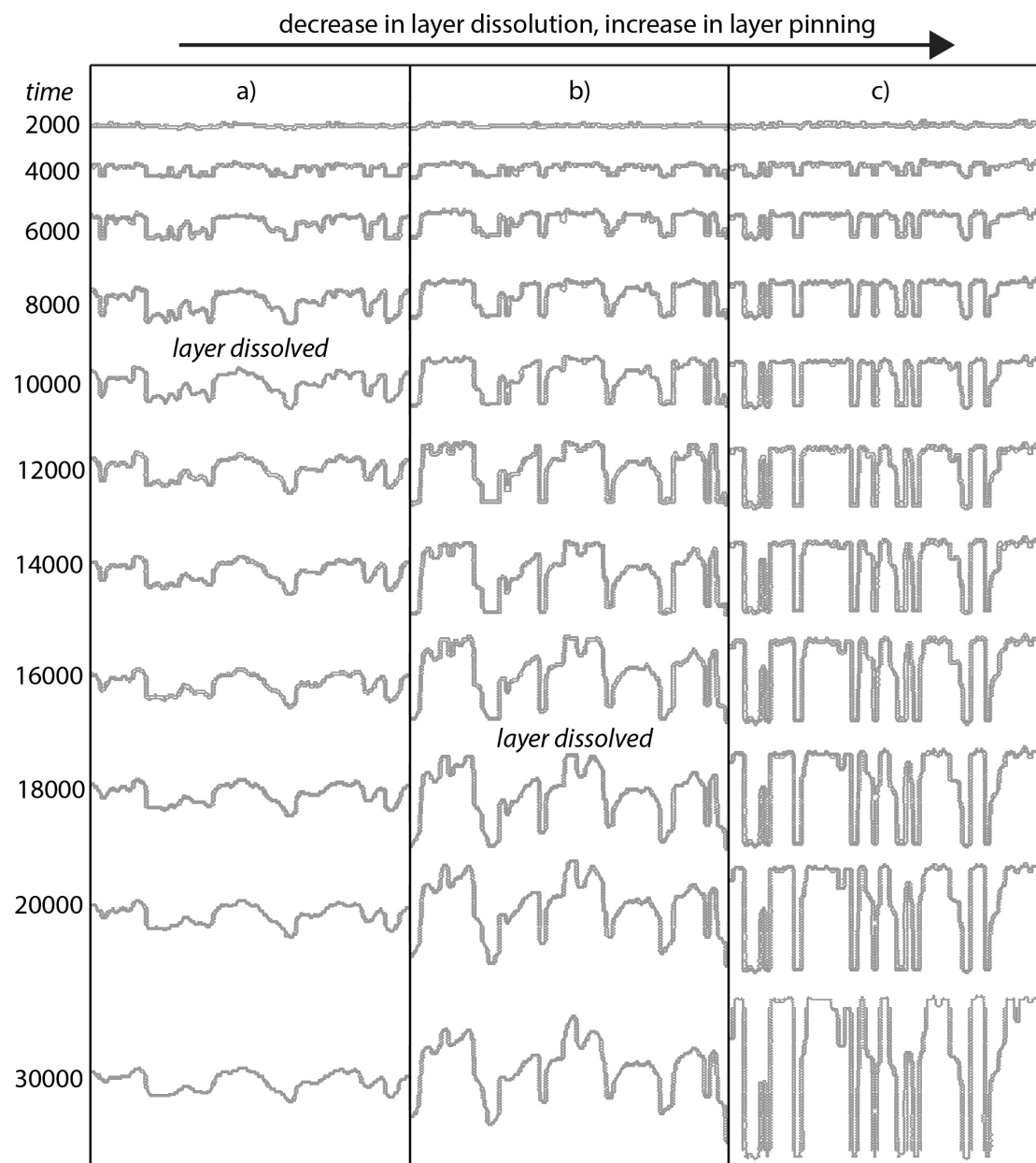


Figure 7 Evolution of three different simulations with initial layer pinning. Layer pinning increases from left to right hand side. If the layer dissolves (cases a and b) the stylolite amplitude growth stops and the corners are rounded. If layer pinning continues (c) the teeth can become very spiky and track almost the full compaction (with the exception of the initial non-linear roughening during the nucleation stage in the layer).

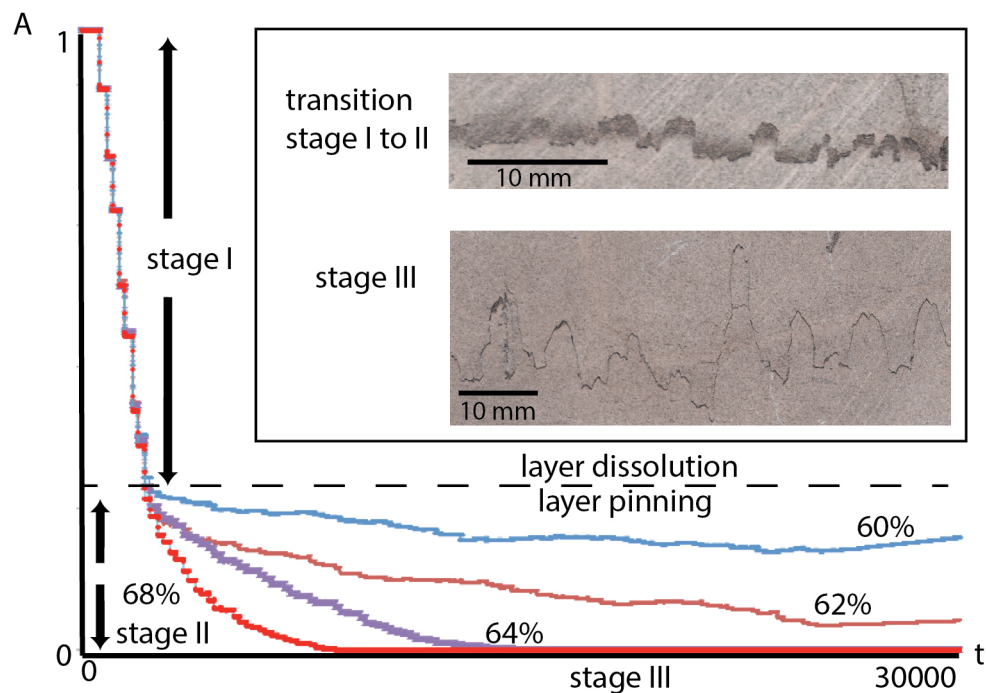


Figure 8 Plot of the dissolution of the layer area (A) versus model time (t) and two stylolite examples. Curves for four different stylolites are shown with a variable dissolution constant of the layer, where the layer dissolves with a rate constant of 60% to 68% of the matrix. The dissolution takes place in three distinct stages. Stage I represents the initial roughening of the stylolite within the layer with non-linear growth and loss of layer material. All stylolites behave the same during this stage. Stage II represents the pinning stage with very slow loss of layer material and linear growth. Strongly pinning layer stylolites remain in this stage (layer factor 60% to 62%). If the layer dissolves the stylolite enters stage III and amplitude growth “freezes”. Two natural stylolite examples are given in the inset. The upper stylolite shows layer remnants on the upper and lower sides of teeth with exactly the same geometry than those of the numerical model in figure 6. This stylolite is at the transition from the initial nucleation to pinning and fast growth. The lower stylolite in the inset has only very minor remnants of layers at peaks and shows otherwise a relatively round roughness. This stylolite is typical of stage III, where the corners are smoothed but amplitude growth freezes.

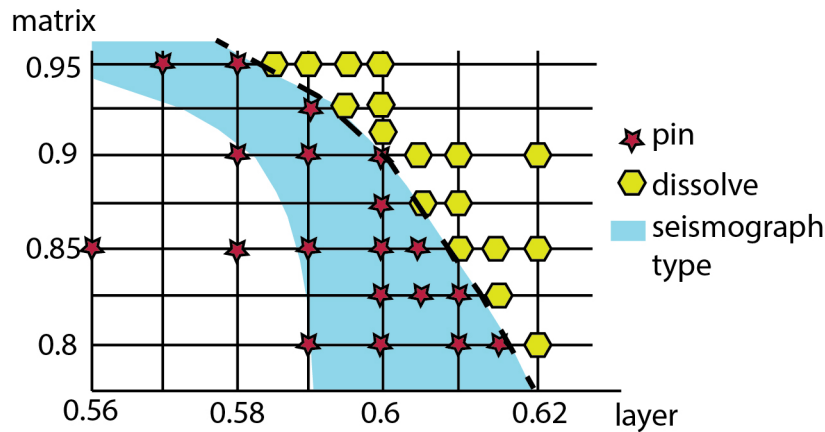


Figure 9 Graph showing pinning strength of the matrix versus pinning strength of the layer. Pinning strength is represented by a linear factor that is multiplied by the dissolution rate of each particle (1 represents 0 pinning strength). For the matrix 10% of particles dissolve a factor x times the dissolution-rate of the matrix. For the layer all particles in the layer dissolve a factor x times the dissolution-rate of the matrix (The layer also contains 10% of particles that dissolve slower than the rest of the layer). The relationship is non-linear where a smaller pinning strength is needed for the layer if the matrix pins more, whereas higher pinning strength is need if the matrix noise is low. A relatively large transition zone exists where seismograph type stylolites can develop that have only partly layer pinning.

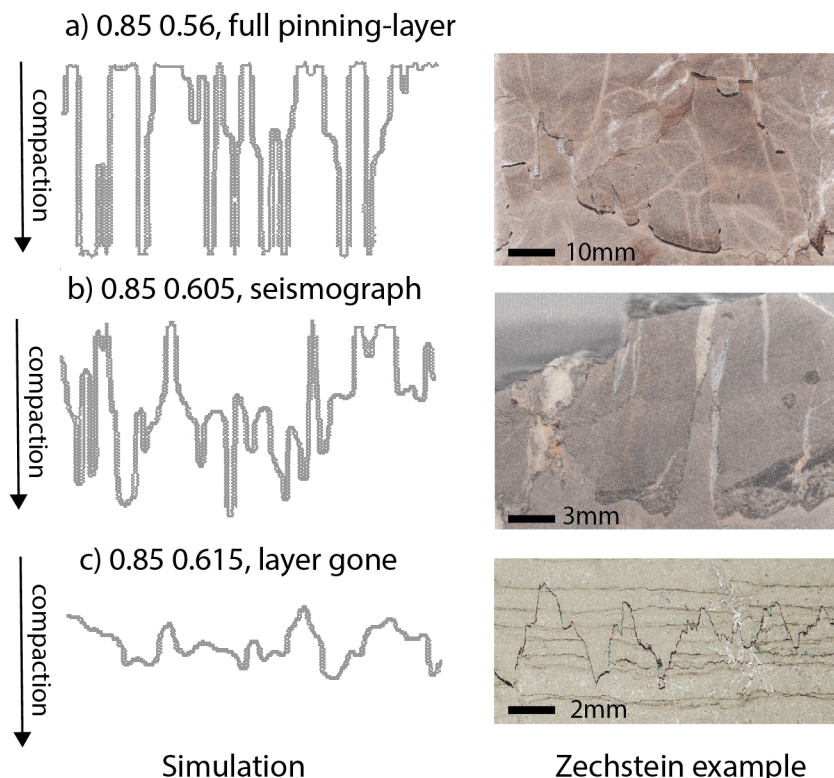
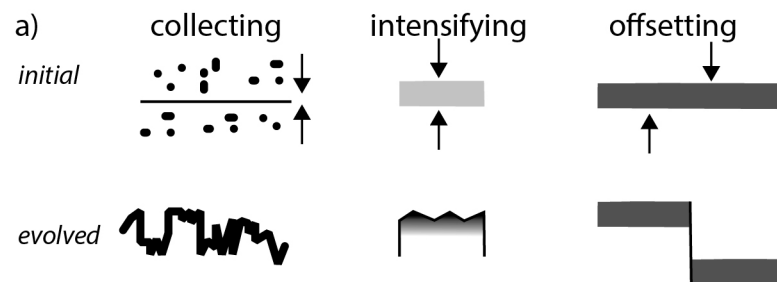


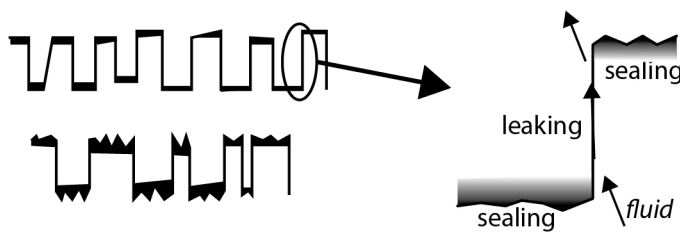
Figure 10 Three distinct stylolite shapes that develop in the model and their counterparts in the Zechstein cores are shown. The first number in the headings represents the matrix noise and the second number the layer pinning strength (with 1.0 meaning no pinning). a) full pinning results in extreme spikes. b) if only parts of the layers survive seismograph stylolites develop. c) once the layer

dissolves completely, the resulting stylolites have an unusual shape and are not growing any more, even if dissolution/compaction continues. The amplitudes cannot grow but the teeth become rounder.

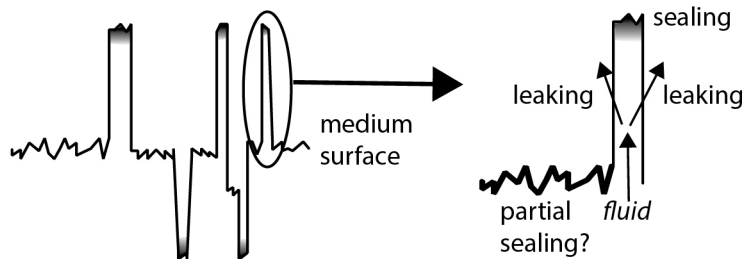


b) Classification

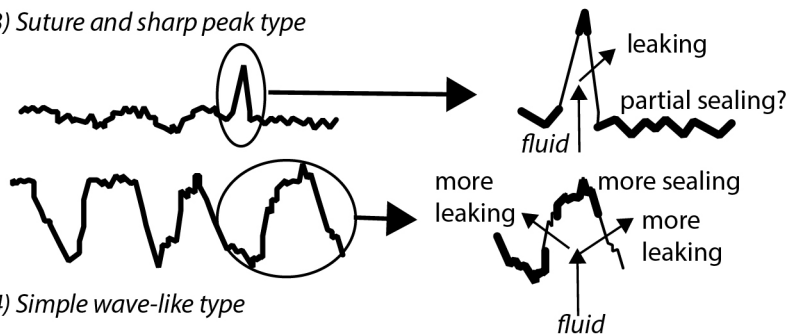
1) Rectangular layer-type with residue layer



2) Seismogram pinning type with a very variable roughness



3) Suture and sharp peak type



4) Simple wave-like type



Figure 11 figure showing an advanced classification of stylolites based on the numerical models and stylolite growth dynamics. a) stylolites can in general either collect material (which may be sealing), intensify densities of material at the top and bottom of teeth (increasing local sealing potential) or offset layers and thus destroying seals. b) advanced classification based on Parks and Schot (1968). 4 types of stylolites are distinguished: 1) rectangular layer type, 2)

seismogram pinning type, 3) suture and sharp peak type and 4) simple wave-like type. The shapes of the different stylolites are shown on the left hand side based on the numerical simulations, whereas the right hand side illustrates the local heterogeneity of permeability across the different types (assuming that the material that the stylolite collects is sealing). Rectangular layer type stylolites offset seals so that the flanks leak whereas the top and bottom of teeth are barriers. Seismogram pinning type offset seals but may collect material and thus seal at median surfaces. They leak across the steep teeth. Suture/sharp peak type collect material that may seal but may leak at sharp peaks and teeth. Simple wave-like type seal if enough material is present or collected, they do not have structures that offset the seals.

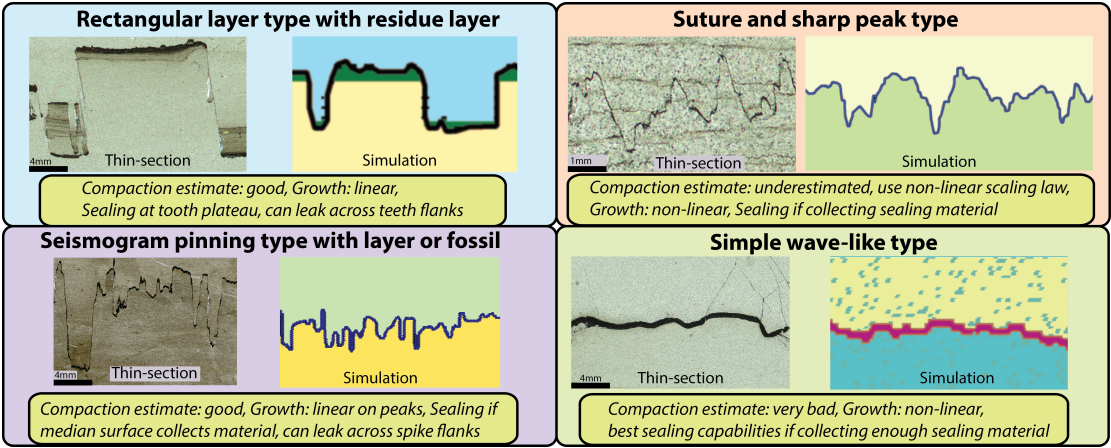


Figure 12 Comparison of natural examples and numerical models of the 4 proposed stylolite types and indications on their capacity to estimate compaction and their influence on local sealing.